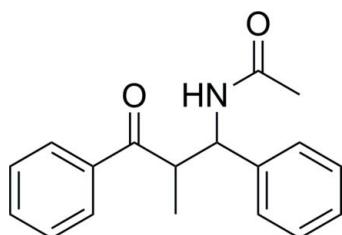


N-(2-Methyl-3-oxo-1,3-diphenylpropyl)-acetamide**Deli Yang, Daxin Shi, Qi Zhang, Hongxin Chai and Jiarong Li***School of Chemical Engineering and Environment, Beijing Institute of Technology, Beijing 100081, People's Republic of China
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Key indicators: single-crystal X-ray study; $T = 153\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$; R factor = 0.070; wR factor = 0.156; data-to-parameter ratio = 15.4.In the title compound, $\text{C}_{18}\text{H}_{19}\text{NO}_2$, the dihedral angle between the benzene rings is $42.0(1)^\circ$. In the crystal, molecules are linked by $\text{N}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\pi$ interactions.**Related literature**For the biological properties of *N*-(2-methyl-3-oxo-1,3-diphenylpropyl)acetamide derivatives, see: Barluenga *et al.* (1993); Casimir *et al.* (1995) and for their synthesis, see: Dakin & West (1928); Selvam & Perumal (2009); Heravi *et al.* (2009).**Experimental***Crystal data*

$\text{C}_{18}\text{H}_{19}\text{NO}_2$
 $M_r = 281.34$
 Monoclinic, $P2_1/c$
 $a = 9.156(5)\text{ \AA}$
 $b = 17.668(8)\text{ \AA}$
 $c = 10.103(5)\text{ \AA}$
 $\beta = 107.914(7)^\circ$

$V = 1555.0(13)\text{ \AA}^3$
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.08\text{ mm}^{-1}$
 $T = 153\text{ K}$
 $0.61 \times 0.07 \times 0.02\text{ mm}$

Data collection

Rigaku AFC10/Saturn724+ diffractometer
 Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2008)
 $T_{\min} = 0.954$, $T_{\max} = 0.998$

12600 measured reflections
 3028 independent reflections
 2386 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.050$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.070$
 $wR(F^2) = 0.156$
 $S = 1.00$
 3028 reflections
 197 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.22\text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.24\text{ e \AA}^{-3}$

Table 1Hydrogen-bond geometry (\AA , $^\circ$).

Cg1 and Cg2 are the centroids of the C10–C15 and C1–C6 benzene rings, respectively.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
N1–H1N \cdots O2 ⁱ	0.94 (3)	1.98 (3)	2.874 (3)	158 (2)
C1–H1 \cdots Cg1 ⁱ	0.95	2.85 (1)	3.649 (3)	142 (1)
C16–H16A \cdots Cg2 ⁱⁱ	0.98	2.98 (1)	3.472 (3)	112 (1)

Symmetry codes: (i) $x, -y + \frac{3}{2}, z - \frac{1}{2}$; (ii) $-x + 1, y + \frac{1}{2}, -z + \frac{3}{2}$.Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure* (Rigaku/MSC, 2009); software used to prepare material for publication: *CrystalStructure*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2279).

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supplementary materials

Acta Cryst. (2013). **E69**, o633 [doi:10.1107/S1600536813007320]

N-(2-Methyl-3-oxo-1,3-diphenylpropyl)acetamide

Deli Yang, Daxin Shi, Qi Zhang, Hongxin Chai and Jiarong Li

Comment

N-(2-methyl-3-oxo-1,3-diphenylpropyl)acetamide is a class of 2-acetamino carbonyl compounds which exhibit great importance of biological (Casimir *et al.*, 1995) and pharmacological (Barluenga *et al.*, 1993) properties. Here, we report the crystal structure of the title compound. In the title molecule (Fig. 1), the dihedral angle formed by the benzene rings is 42.0°, and the methyl and the acetamide groups have an anti-conformation. In the crystal structure (Fig. 2), molecules are connected by N—H···O and C—H···π interactions (Table 1, Cg1 and Cg2 are the centroids of the C10–C15 benzene ring and the C1–C6 benzene ring, respectively).

Experimental

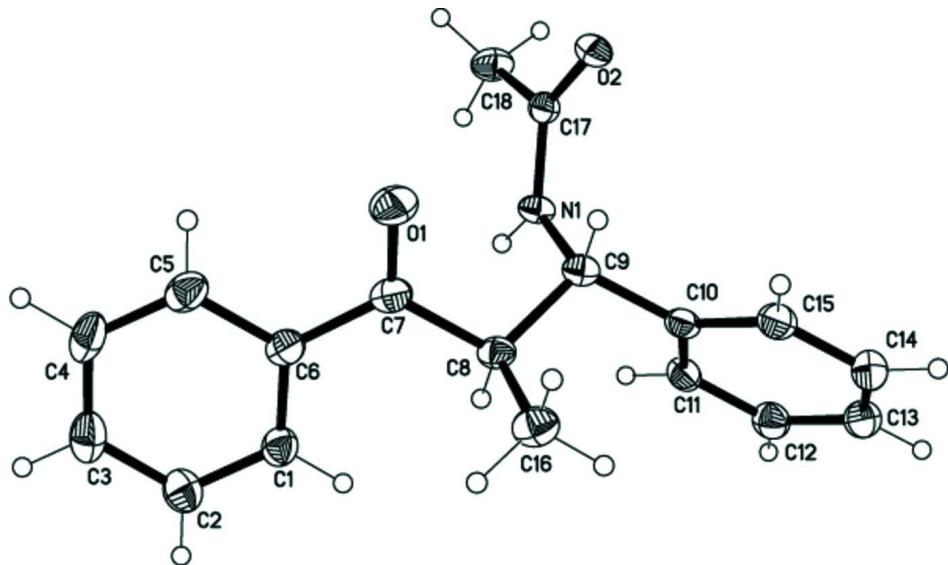
A solution of benzaldehyde (2 mmol) and propiophenone (2 mmol) in the presence of acetyl chloride and TiCl_4 was stirred in acetonitrile (5 ml) at room temperature for 3 h. The reaction mixture was poured to room temperature and then filtered to give the title compound. The product was recrystallized from petroleum ether and ethyl acetate to give white crystalline powder. m.p. 439–441 K.

Refinement

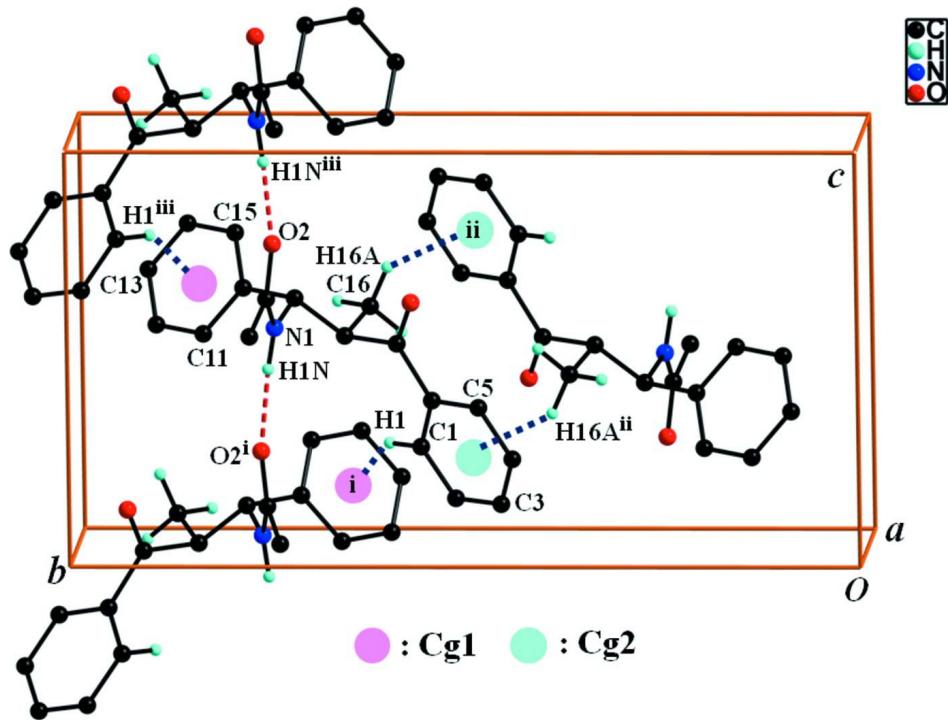
C—H were included in the riding model approximation with C—H distances 0.95–1.00 Å, and with $U_{\text{iso}}(\text{H})=1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{C})(\text{methyl})$. Freely refined H atoms of NH group were located in difference Fourier maps with N—H distances 0.94 Å with $U_{\text{iso}}(\text{H})=1.5U_{\text{eq}}(\text{N})$.

Computing details

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear* (Rigaku, 2008); data reduction: *CrystalClear* (Rigaku, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure* (Rigaku/MSC, 2009); software used to prepare material for publication: *CrystalStructure* (Rigaku/MSC, 2009).

**Figure 1**

The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

**Figure 2**

A view of N—H···O and C—H···π interactions. (dotted lines) in the crystal structure of the title compound. H atoms non-participating in hydrogen-bonding were omitted for clarity. [Symmetry codes: (i) $x, -y + 3/2, z - 1/2$; (ii) $-x + 1, -y + 1, -z + 1$; (iii) $x, -y + 3/2, z + 1/2$.]

N*-(2-Methyl-3-oxo-1,3-diphenylpropyl)acetamideCrystal data*

$C_{18}H_{19}NO_2$
 $M_r = 281.34$
 Monoclinic, $P2_1/c$
 Hall symbol: -P 2ybc
 $a = 9.156$ (5) Å
 $b = 17.668$ (8) Å
 $c = 10.103$ (5) Å
 $\beta = 107.914$ (7)°
 $V = 1555.0$ (13) Å³
 $Z = 4$

$F(000) = 600$
 $D_x = 1.202$ Mg m⁻³
 Melting point = 439–441 K
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 3372 reflections
 $\theta = 2.3\text{--}29.0^\circ$
 $\mu = 0.08$ mm⁻¹
 $T = 153$ K
 Prism, colorless
 $0.61 \times 0.07 \times 0.02$ mm

Data collection

Rigaku AFC10/Saturn724+
 diffractometer
 Radiation source: Rotating Anode
 Graphite monochromator
 Detector resolution: 28.5714 pixels mm⁻¹
 phi and ω scans
 Absorption correction: multi-scan
 (*CrystalClear*; Rigaku, 2008)
 $T_{\min} = 0.954$, $T_{\max} = 0.998$

12600 measured reflections
 3028 independent reflections
 2386 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.050$
 $\theta_{\max} = 26.0^\circ$, $\theta_{\min} = 2.3^\circ$
 $h = -11 \rightarrow 11$
 $k = -20 \rightarrow 21$
 $l = -12 \rightarrow 12$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.070$
 $wR(F^2) = 0.156$
 $S = 1.00$
 3028 reflections
 197 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods
 Secondary atom site location: difference Fourier
 map

Hydrogen site location: difference Fourier map
 H atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 1.630P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.22$ e Å⁻³
 $\Delta\rho_{\min} = -0.24$ e Å⁻³
 Extinction correction: *SHELXL97* (Sheldrick,
 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.014 (2)

Special details

Experimental. Spectral data: IR (KBr): 3297, 3061, 2980, 1683, 1651, 1544, 1448, 1370, 1208, 1140, 970, 707, 615 cm⁻¹; ¹H-NMR(DMSO,p.p.m.):1.13 (3H, d, $J = 6.8$ Hz C₁H₃), 1.85 (3H, s, C₁O₁C₁H₃), 4.00–4.14 (1H, m, C₁H₁), 5.26 (1H, t, $J = 11.6$ Hz, C₁H₁), 7.12 (1H, t, $J = 6.8$ Hz, Benzene-H), 7.22 (2H, t, $J = 8.0$ Hz, Benzene-H), 7.29 (2H, d, $J = 7.6$ Hz, Benzene-H), 7.47 (2H, t, $J = 8.0$ Hz, Benzene-H), 7.58 (1H, t, $J = 6.8$ Hz, Benzene-H), 7.80 (2H, t, $J = 7.6$ Hz, Benzene-H), 8.30 (1H, d, $J = 9.2$ Hz, NH); ESI-MS m/z: [M⁺Na]⁺ 304.2.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.2368 (2)	0.56897 (11)	0.6152 (2)	0.0553 (6)
O2	0.13769 (19)	0.74116 (10)	0.76594 (17)	0.0390 (4)
N1	0.1849 (2)	0.74059 (11)	0.5589 (2)	0.0305 (5)
C1	0.2662 (3)	0.55877 (14)	0.2653 (3)	0.0401 (6)
H1	0.3342	0.5998	0.2680	0.048*
C2	0.2150 (3)	0.51473 (15)	0.1457 (3)	0.0483 (7)
H2	0.2490	0.5252	0.0677	0.058*
C3	0.1143 (3)	0.45551 (16)	0.1410 (3)	0.0535 (8)
H3	0.0791	0.4255	0.0593	0.064*
C4	0.0646 (3)	0.43978 (15)	0.2540 (3)	0.0520 (8)
H4	-0.0055	0.3995	0.2497	0.062*
C5	0.1172 (3)	0.48288 (15)	0.3731 (3)	0.0456 (7)
H5	0.0841	0.4714	0.4512	0.055*
C6	0.2190 (3)	0.54355 (13)	0.3808 (3)	0.0373 (6)
C7	0.2732 (3)	0.58798 (14)	0.5128 (3)	0.0384 (6)
C8	0.3799 (3)	0.65579 (13)	0.5217 (2)	0.0324 (5)
H8	0.3626	0.6769	0.4263	0.039*
C9	0.3469 (3)	0.71774 (13)	0.6157 (2)	0.0317 (5)
H9	0.3627	0.6956	0.7101	0.038*
C10	0.4548 (3)	0.78490 (13)	0.6304 (2)	0.0327 (5)
C11	0.4362 (3)	0.83580 (13)	0.5211 (3)	0.0369 (6)
H11	0.3546	0.8289	0.4372	0.044*
C12	0.5363 (3)	0.89691 (15)	0.5338 (3)	0.0444 (7)
H12	0.5236	0.9308	0.4580	0.053*
C13	0.6541 (3)	0.90834 (16)	0.6565 (3)	0.0472 (7)
H13	0.7209	0.9505	0.6656	0.057*
C14	0.6741 (3)	0.85819 (16)	0.7654 (3)	0.0470 (7)
H14	0.7551	0.8657	0.8495	0.056*
C15	0.5756 (3)	0.79640 (15)	0.7523 (3)	0.0400 (6)
H15	0.5910	0.7618	0.8273	0.048*
C16	0.5456 (3)	0.62634 (15)	0.5778 (3)	0.0439 (6)
H16A	0.5626	0.6044	0.6704	0.053*
H16B	0.6174	0.6683	0.5838	0.053*
H16C	0.5626	0.5875	0.5148	0.053*
C17	0.0921 (3)	0.74884 (12)	0.6372 (2)	0.0304 (5)
C18	-0.0729 (3)	0.76761 (16)	0.5617 (3)	0.0443 (7)
H18A	-0.1391	0.7270	0.5764	0.053*
H18B	-0.0867	0.7728	0.4621	0.053*
H18C	-0.1003	0.8153	0.5976	0.053*
H1N	0.143 (3)	0.7487 (15)	0.463 (3)	0.045 (8)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0705 (14)	0.0501 (12)	0.0574 (12)	-0.0110 (10)	0.0374 (11)	0.0049 (9)
O2	0.0429 (10)	0.0491 (11)	0.0273 (9)	-0.0032 (8)	0.0144 (7)	-0.0034 (7)
N1	0.0310 (10)	0.0378 (11)	0.0252 (10)	0.0059 (8)	0.0122 (8)	0.0044 (8)

C1	0.0411 (14)	0.0314 (13)	0.0484 (15)	-0.0016 (11)	0.0149 (12)	-0.0001 (11)
C2	0.0540 (16)	0.0398 (15)	0.0507 (17)	0.0019 (13)	0.0157 (14)	-0.0025 (12)
C3	0.0512 (16)	0.0361 (15)	0.065 (2)	-0.0022 (13)	0.0063 (15)	-0.0054 (13)
C4	0.0422 (15)	0.0315 (14)	0.078 (2)	-0.0072 (12)	0.0126 (15)	0.0000 (13)
C5	0.0415 (15)	0.0352 (14)	0.0650 (19)	0.0015 (11)	0.0236 (14)	0.0066 (12)
C6	0.0362 (13)	0.0276 (12)	0.0517 (15)	0.0044 (10)	0.0190 (12)	0.0039 (10)
C7	0.0386 (13)	0.0340 (13)	0.0480 (15)	0.0036 (11)	0.0216 (12)	0.0056 (11)
C8	0.0364 (12)	0.0302 (12)	0.0347 (12)	0.0023 (10)	0.0172 (10)	0.0055 (9)
C9	0.0321 (12)	0.0359 (13)	0.0291 (12)	0.0045 (10)	0.0121 (10)	0.0036 (9)
C10	0.0336 (12)	0.0361 (13)	0.0319 (12)	0.0035 (10)	0.0151 (10)	-0.0036 (10)
C11	0.0459 (14)	0.0335 (13)	0.0340 (13)	-0.0012 (11)	0.0163 (11)	-0.0043 (10)
C12	0.0546 (16)	0.0338 (14)	0.0499 (16)	-0.0018 (12)	0.0235 (14)	-0.0036 (11)
C13	0.0499 (16)	0.0396 (15)	0.0576 (17)	-0.0069 (12)	0.0245 (14)	-0.0101 (13)
C14	0.0425 (15)	0.0511 (17)	0.0470 (16)	-0.0064 (13)	0.0132 (12)	-0.0118 (13)
C15	0.0383 (13)	0.0471 (15)	0.0357 (13)	0.0031 (11)	0.0131 (11)	-0.0022 (11)
C16	0.0406 (14)	0.0395 (14)	0.0545 (17)	0.0083 (12)	0.0190 (13)	0.0072 (12)
C17	0.0347 (12)	0.0273 (11)	0.0312 (12)	-0.0021 (9)	0.0129 (10)	-0.0013 (9)
C18	0.0363 (13)	0.0554 (17)	0.0446 (15)	0.0087 (12)	0.0172 (12)	0.0066 (12)

Geometric parameters (\AA , $^\circ$)

O1—C7	1.227 (3)	C9—C10	1.522 (3)
O2—C17	1.245 (3)	C9—H9	1.0000
N1—C17	1.336 (3)	C10—C11	1.393 (3)
N1—C9	1.473 (3)	C10—C15	1.394 (3)
N1—H1N	0.94 (3)	C11—C12	1.396 (4)
C1—C6	1.390 (3)	C11—H11	0.9500
C1—C2	1.392 (4)	C12—C13	1.385 (4)
C1—H1	0.9500	C12—H12	0.9500
C2—C3	1.386 (4)	C13—C14	1.380 (4)
C2—H2	0.9500	C13—H13	0.9500
C3—C4	1.381 (4)	C14—C15	1.396 (4)
C3—H3	0.9500	C14—H14	0.9500
C4—C5	1.380 (4)	C15—H15	0.9500
C4—H4	0.9500	C16—H16A	0.9800
C5—C6	1.407 (3)	C16—H16B	0.9800
C5—H5	0.9500	C16—H16C	0.9800
C6—C7	1.494 (4)	C17—C18	1.505 (3)
C7—C8	1.531 (3)	C18—H18A	0.9800
C8—C16	1.538 (3)	C18—H18B	0.9800
C8—C9	1.538 (3)	C18—H18C	0.9800
C8—H8	1.0000		
C17—N1—C9	123.2 (2)	C8—C9—H9	108.2
C17—N1—H1N	117.8 (16)	C11—C10—C15	118.4 (2)
C9—N1—H1N	119.0 (16)	C11—C10—C9	120.5 (2)
C6—C1—C2	120.8 (3)	C15—C10—C9	121.0 (2)
C6—C1—H1	119.6	C10—C11—C12	120.6 (2)
C2—C1—H1	119.6	C10—C11—H11	119.7
C3—C2—C1	119.6 (3)	C12—C11—H11	119.7

C3—C2—H2	120.2	C13—C12—C11	120.2 (3)
C1—C2—H2	120.2	C13—C12—H12	119.9
C4—C3—C2	120.6 (3)	C11—C12—H12	119.9
C4—C3—H3	119.7	C14—C13—C12	119.7 (3)
C2—C3—H3	119.7	C14—C13—H13	120.2
C5—C4—C3	119.6 (3)	C12—C13—H13	120.2
C5—C4—H4	120.2	C13—C14—C15	120.2 (3)
C3—C4—H4	120.2	C13—C14—H14	119.9
C4—C5—C6	121.1 (3)	C15—C14—H14	119.9
C4—C5—H5	119.4	C10—C15—C14	120.8 (3)
C6—C5—H5	119.4	C10—C15—H15	119.6
C1—C6—C5	118.2 (2)	C14—C15—H15	119.6
C1—C6—C7	123.0 (2)	C8—C16—H16A	109.5
C5—C6—C7	118.9 (2)	C8—C16—H16B	109.5
O1—C7—C6	120.4 (2)	H16A—C16—H16B	109.5
O1—C7—C8	119.9 (2)	C8—C16—H16C	109.5
C6—C7—C8	119.6 (2)	H16A—C16—H16C	109.5
C7—C8—C16	107.2 (2)	H16B—C16—H16C	109.5
C7—C8—C9	110.49 (19)	O2—C17—N1	122.5 (2)
C16—C8—C9	111.9 (2)	O2—C17—C18	121.0 (2)
C7—C8—H8	109.1	N1—C17—C18	116.5 (2)
C16—C8—H8	109.1	C17—C18—H18A	109.5
C9—C8—H8	109.1	C17—C18—H18B	109.5
N1—C9—C10	111.73 (19)	H18A—C18—H18B	109.5
N1—C9—C8	108.67 (19)	C17—C18—H18C	109.5
C10—C9—C8	111.73 (18)	H18A—C18—H18C	109.5
N1—C9—H9	108.2	H18B—C18—H18C	109.5
C10—C9—H9	108.2		
C6—C1—C2—C3	0.8 (4)	C7—C8—C9—N1	−58.1 (2)
C1—C2—C3—C4	−0.1 (4)	C16—C8—C9—N1	−177.54 (19)
C2—C3—C4—C5	−0.8 (4)	C7—C8—C9—C10	178.12 (19)
C3—C4—C5—C6	1.0 (4)	C16—C8—C9—C10	58.7 (3)
C2—C1—C6—C5	−0.5 (4)	N1—C9—C10—C11	−47.8 (3)
C2—C1—C6—C7	178.6 (2)	C8—C9—C10—C11	74.1 (3)
C4—C5—C6—C1	−0.4 (4)	N1—C9—C10—C15	133.1 (2)
C4—C5—C6—C7	−179.5 (2)	C8—C9—C10—C15	−104.9 (2)
C1—C6—C7—O1	−174.8 (2)	C15—C10—C11—C12	−0.1 (3)
C5—C6—C7—O1	4.3 (4)	C9—C10—C11—C12	−179.2 (2)
C1—C6—C7—C8	2.8 (3)	C10—C11—C12—C13	−1.1 (4)
C5—C6—C7—C8	−178.0 (2)	C11—C12—C13—C14	1.3 (4)
O1—C7—C8—C16	86.0 (3)	C12—C13—C14—C15	−0.3 (4)
C6—C7—C8—C16	−91.6 (3)	C11—C10—C15—C14	1.0 (4)
O1—C7—C8—C9	−36.1 (3)	C9—C10—C15—C14	−179.9 (2)
C6—C7—C8—C9	146.2 (2)	C13—C14—C15—C10	−0.9 (4)
C17—N1—C9—C10	−102.4 (2)	C9—N1—C17—O2	3.4 (3)
C17—N1—C9—C8	133.9 (2)	C9—N1—C17—C18	−176.2 (2)

Hydrogen-bond geometry (Å, °)

Cg1 and Cg2 are the centroids of the C10–C15 and C1–C6 benzene rings, respectively.

$D\text{—H}\cdots A$	$D\text{—H}$	$\text{H}\cdots A$	$D\cdots A$	$D\text{—H}\cdots A$
N1—H1N \cdots O2 ⁱ	0.94 (3)	1.98 (3)	2.874 (3)	158 (2)
C1—H1 \cdots Cg1 ⁱ	0.95	2.85 (1)	3.649 (3)	142 (1)
C16—H16A \cdots Cg2 ⁱⁱ	0.98	2.98 (1)	3.472 (3)	112 (1)

Symmetry codes: (i) $x, -y+3/2, z-1/2$; (ii) $-x+1, y+3/2, -z+3/2$.